



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 03:37 PM GMT

PDB ID : 2Q7X  
Title : Crystal structure of a putative phospho transferase (sp\_1565) from streptococcus pneumoniae tigr4 at 2.00 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2007-06-07  
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

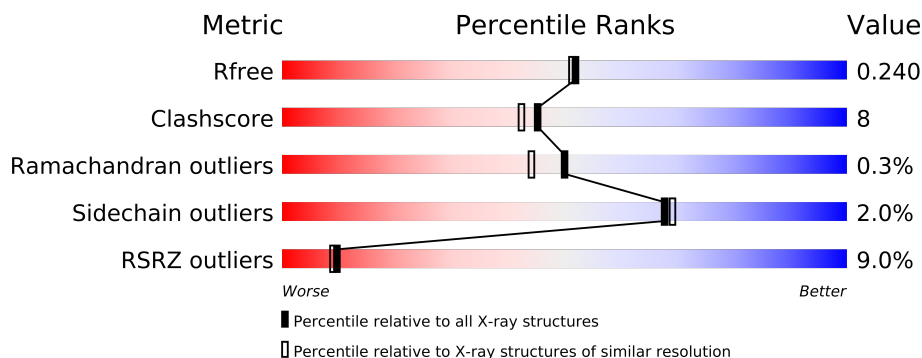
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	326	
1	B	326	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	PEG	A	328	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5147 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called UPF0052 protein SP\_1565.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	Se	0	5	0
			2465	1560	419	474	2	10			
1	B	305	Total	C	N	O	S	Se	0	7	0
			2385	1516	408	451	2	8			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP Q97PN8
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	3	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	5	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	20	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	25	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	47	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	49	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	65	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	68	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	70	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	74	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	103	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	111	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	116	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	123	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	186	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	205	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	215	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	225	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	261	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	267	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	288	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
A	318	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
A	324	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	0	GLY	-	LEADER SEQUENCE	UNP Q97PN8
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	3	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	5	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	20	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	25	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	47	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	49	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	65	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	68	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	70	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	74	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	103	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	111	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	116	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	123	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	186	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	205	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	215	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	225	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	261	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	267	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	288	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	318	MSE	MET	MODIFIED RESIDUE	UNP Q97PN8
B	324	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8
B	325	MLY	LYS	MODIFIED RESIDUE	UNP Q97PN8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is water.

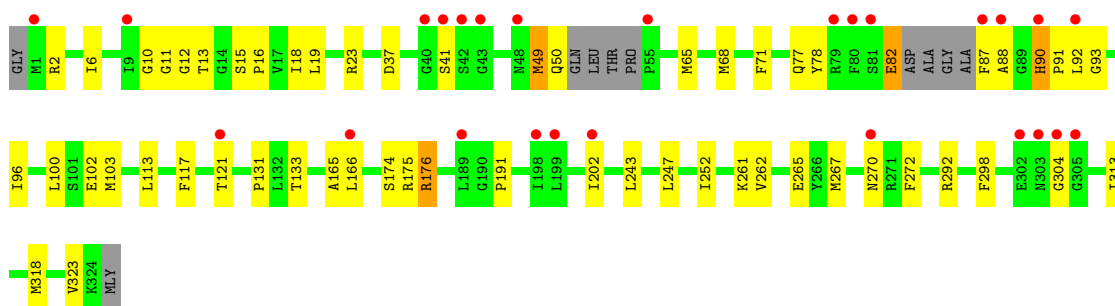
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	163	Total	O	0	0
			163	163		
4	B	119	Total	O	0	0
			119	119		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

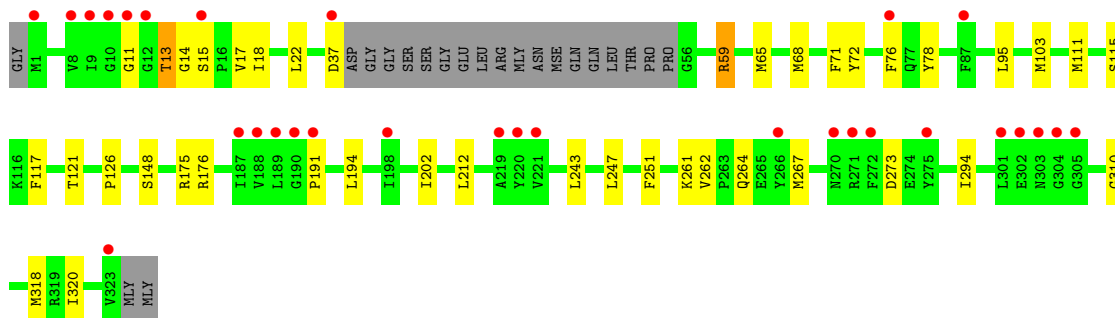
- Molecule 1: UPF0052 protein SP\_1565

Chain A: 



- Molecule 1: UPF0052 protein SP\_1565

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.52Å 69.35Å 169.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 2.00 29.55 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.55-2.00) 99.7 (29.55-2.00)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.195 , 0.236 0.198 , 0.240	Depositor DCC
$R_{free}$ test set	2656 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.1	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 59.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 52112 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5147	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, MLY, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.83	0/2380	0.84	2/3221 (0.1%)
1	B	0.70	0/2310	0.75	0/3132
All	All	0.77	0/4690	0.80	2/6353 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	A	292	ARG	NE-CZ-NH2	-8.09	116.25	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	ARG	Peptide
1	B	13	THR	Peptide



## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2465	0	2395	46	0
1	B	2385	0	2330	44	0
2	A	1	0	0	0	0
3	A	14	0	20	0	0
4	A	163	0	0	1	0
4	B	119	0	0	0	0
All	All	5147	0	4745	81	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (81) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:212:LEU:HD21	1:B:247[A]:LEU:CD2	1.98	0.93
1:B:11[B]:GLY:HA2	1:B:191:PRO:O	1.71	0.88
1:A:261:MLY:HH13	1:A:267:MSE:HE1	1.55	0.87
1:A:103:MSE:HE2	1:B:78:TYR:HB2	1.67	0.74
1:A:90:HIS:ND1	1:A:91:PRO:HD2	2.02	0.74
1:B:175:ARG:O	1:B:176:ARG:HB2	1.89	0.73
1:A:18:ILE:HD12	1:A:191:PRO:HD3	1.70	0.73
1:A:261:MLY:HH12	1:A:262:VAL:O	1.89	0.72
1:A:270:ASN:OD1	1:A:304:GLY:HA2	1.91	0.71
1:B:261:MLY:HH12	1:B:267:MSE:HE1	1.74	0.70
1:B:212:LEU:CD2	1:B:247[A]:LEU:HD21	2.22	0.69
1:B:262:VAL:O	1:B:267:MSE:HE2	1.92	0.69
1:B:212:LEU:CG	1:B:247[A]:LEU:HD21	2.23	0.68
1:B:212:LEU:HD21	1:B:247[A]:LEU:HD21	1.75	0.68
1:A:92:LEU:HD23	1:A:93:GLY:N	2.10	0.67
1:A:82:GLU:OE2	1:A:87:PHE:N	2.28	0.67
1:A:68:MSE:HE3	1:A:71:PHE:CD2	2.30	0.67
1:B:212:LEU:HG	1:B:247[A]:LEU:HD21	1.77	0.66
1:A:37:ASP:OD1	1:A:133:THR:HG23	1.96	0.66
1:B:212:LEU:HD21	1:B:247[A]:LEU:HD22	1.76	0.66
1:A:18:ILE:HD12	1:A:191:PRO:CD	2.27	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:261:MLY:CH1	1:A:267:MSE:HE1	2.25	0.65
1:A:243:LEU:HD13	1:A:252:ILE:HD11	1.78	0.63
1:B:68:MSE:HE3	1:B:71:PHE:CD2	2.35	0.61
1:A:298:PHE:CD1	1:A:313:ILE:HD13	2.35	0.61
1:A:87:PHE:HB3	1:A:88:ALA:HA	1.82	0.60
1:B:22:LEU:HD23	1:B:318:MSE:CE	2.32	0.60
1:A:2:ARG:NH2	1:A:323:VAL:HG13	2.17	0.59
1:A:96:ILE:O	1:A:100:LEU:HD13	2.05	0.57
1:A:41:SER:OG	1:A:166:LEU:HD21	2.06	0.55
1:B:294:ILE:HD11	1:B:320:ILE:HD11	1.88	0.55
1:B:13:THR:N	1:B:14:GLY:HA3	2.22	0.55
1:B:212:LEU:CD2	1:B:247[A]:LEU:CD2	2.75	0.54
1:A:267:MSE:HG2	1:A:272:PHE:CD2	2.44	0.52
1:A:18:ILE:CD1	1:A:191:PRO:HD3	2.40	0.52
1:B:72:TYR:O	1:B:76:PHE:HB2	2.10	0.51
1:A:113:LEU:HD22	1:B:71:PHE:HE1	1.75	0.50
1:B:202:ILE:O	1:B:247[B]:LEU:HD21	2.11	0.50
1:B:247[A]:LEU:HD23	1:B:247[A]:LEU:O	2.11	0.50
1:B:17:VAL:HG12	1:B:310:GLY:HA3	1.93	0.49
1:B:294:ILE:CD1	1:B:320:ILE:HD11	2.43	0.49
1:A:131:PRO:HB2	1:A:165:ALA:HB3	1.96	0.48
1:A:102:GLU:OE1	1:B:78:TYR:OH	2.21	0.48
1:A:78:TYR:CB	1:B:103:MSE:HE2	2.44	0.48
1:A:6:ILE:HD11	1:A:318:MSE:HE1	1.95	0.48
1:B:11[B]:GLY:HA3	1:B:15[B]:SER:OG	2.13	0.48
1:B:264:GLN:HA	1:B:267:MSE:HE3	1.96	0.48
1:A:78:TYR:HB3	1:B:103:MSE:HE2	1.95	0.47
1:A:174:SER:O	1:A:176:ARG:HG2	2.15	0.47
1:A:49:MSE:O	1:A:49:MSE:HG3	2.14	0.46
1:B:22:LEU:HD23	1:B:318:MSE:HE2	1.97	0.45
1:A:113:LEU:HD22	1:B:71:PHE:CE1	2.51	0.45
1:B:202:ILE:HD12	1:B:247[B]:LEU:HG	1.98	0.45
1:B:22:LEU:CD2	1:B:318:MSE:CE	2.95	0.45
1:A:261:MLY:HH13	1:A:267:MSE:CE	2.38	0.45
1:B:111:MSE:CE	1:B:126:PRO:HD3	2.47	0.44
1:A:19:LEU:O	1:A:23:ARG:HG3	2.17	0.44
1:A:96:ILE:HD13	1:A:117:PHE:CZ	2.52	0.44
1:A:10[B]:GLY:O	1:A:12:GLY:N	2.50	0.44
1:B:111:MSE:HE2	1:B:126:PRO:CD	2.48	0.44
1:B:194:LEU:HD11	1:B:243:LEU:HG	2.00	0.43
1:A:87:PHE:CE2	1:B:95:LEU:HD21	2.53	0.43
1:A:65[A]:MSE:HE3	1:A:121:THR:O	2.19	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:49:MSE:O	1:A:50:GLN:HB2	2.18	0.43
1:A:13:THR:CG2	4:A:377:HOH:O	2.66	0.43
1:A:261:MLY:CH1	1:A:262:VAL:O	2.61	0.42
1:B:111:MSE:HE2	1:B:126:PRO:CG	2.49	0.42
1:B:11[A]:GLY:HA3	1:B:15[A]:SER:HB3	1.99	0.42
1:A:65[A]:MSE:O	1:A:121:THR:HG22	2.20	0.42
1:A:202:ILE:HD12	1:A:247:LEU:HB2	2.02	0.42
1:B:273:ASP:C	1:B:273:ASP:OD1	2.58	0.42
1:A:103:MSE:HE2	1:B:78:TYR:CB	2.43	0.41
1:A:6:ILE:CD1	1:A:318:MSE:HE1	2.49	0.41
1:A:15[B]:SER:N	1:A:16:PRO:CD	2.83	0.41
1:B:11[A]:GLY:CA	1:B:15[A]:SER:HB3	2.50	0.41
1:A:267:MSE:HG2	1:A:272:PHE:CE2	2.54	0.41
1:B:65:MSE:HE3	1:B:121:THR:O	2.21	0.41
1:A:15[A]:SER:N	1:A:16:PRO:CD	2.84	0.41
1:B:247[A]:LEU:HD13	1:B:251:PHE:CE1	2.56	0.41
1:A:117:PHE:CZ	1:B:117:PHE:HZ	2.39	0.40
1:B:59[B]:ARG:HG2	1:B:76:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	302/326 (93%)	292 (97%)	8 (3%)	2 (1%)	30	20
1	B	296/326 (91%)	287 (97%)	9 (3%)	0	100	100
All	All	598/652 (92%)	579 (97%)	17 (3%)	2 (0%)	50	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLY
1	A	77	GLN

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/257 (100%)	252 (98%)	6 (2%)	63	63
1	B	246/257 (96%)	240 (98%)	6 (2%)	61	61
All	All	504/514 (98%)	492 (98%)	12 (2%)	68	61

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	MSE
1	A	82	GLU
1	A	90	HIS
1	A	176	ARG
1	A	265[A]	GLU
1	A	265[B]	GLU
1	B	18	ILE
1	B	37	ASP
1	B	59[A]	ARG
1	B	59[B]	ARG
1	B	115	SER
1	B	148	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

26 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	MLY	A	116	1	7,8,11	6.52	2 (28%)	5,8,13	1.22	0
1	MLY	A	123	1	5,5,11	6.90	1 (20%)	2,5,13	2.77	1 (50%)
1	MLY	A	20	1	5,5,11	8.63	2 (40%)	2,5,13	1.62	0
1	MLY	A	205	1	10,10,11	5.53	1 (10%)	9,11,13	1.71	2 (22%)
1	MLY	A	215	1	7,8,11	6.65	1 (14%)	5,8,13	0.94	0
1	MLY	A	25	1	10,10,11	5.79	1 (10%)	9,11,13	2.45	3 (33%)
1	MLY	A	261	1	10,10,11	4.83	1 (10%)	9,11,13	1.93	4 (44%)
1	MLY	A	288	1	7,8,11	5.15	2 (28%)	5,8,13	1.90	1 (20%)
1	MLY	A	3	1	7,8,11	7.01	2 (28%)	5,8,13	1.73	1 (20%)
1	MLY	A	324	1	10,10,11	5.94	2 (20%)	9,11,13	1.76	2 (22%)
1	MLY	A	47	1	3,4,11	10.74	2 (66%)	1,4,13	1.64	0
1	MLY	A	5	1	10,10,11	6.06	2 (20%)	9,11,13	1.81	4 (44%)
1	MLY	A	70	1	5,5,11	8.52	2 (40%)	2,5,13	5.14	1 (50%)
1	MLY	A	74	1	3,4,11	10.45	1 (33%)	1,4,13	5.25	1 (100%)
1	MLY	B	116	1	7,8,11	6.81	1 (14%)	5,8,13	2.00	1 (20%)
1	MLY	B	123	1	10,10,11	5.55	1 (10%)	9,11,13	1.90	4 (44%)
1	MLY	B	20	1	7,8,11	6.62	1 (14%)	5,8,13	0.97	0
1	MLY	B	205	1	6,6,11	6.24	3 (50%)	4,6,13	1.65	2 (50%)
1	MLY	B	215	1	5,5,11	7.55	3 (60%)	2,5,13	0.46	0
1	MLY	B	25	1	10,10,11	5.43	1 (10%)	9,11,13	2.15	3 (33%)
1	MLY	B	261	1	10,10,11	5.08	1 (10%)	9,11,13	2.12	3 (33%)
1	MLY	B	288	1	5,5,11	8.69	3 (60%)	2,5,13	1.27	0
1	MLY	B	3	1	7,8,11	6.36	1 (14%)	5,8,13	2.34	2 (40%)
1	MLY	B	5	1	7,8,11	7.71	1 (14%)	5,8,13	2.75	1 (20%)
1	MLY	B	70	1	10,10,11	5.00	2 (20%)	9,11,13	1.95	4 (44%)
1	MLY	B	74	1	7,8,11	6.87	1 (14%)	5,8,13	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	116	1	-	0/5/7/11	0/0/0/0
1	MLY	A	123	1	-	0/2/4/11	0/0/0/0
1	MLY	A	20	1	-	0/2/4/11	0/0/0/0
1	MLY	A	205	1	-	0/7/9/11	0/0/0/0
1	MLY	A	215	1	-	0/5/7/11	0/0/0/0
1	MLY	A	25	1	-	0/7/9/11	0/0/0/0
1	MLY	A	261	1	-	0/7/9/11	0/0/0/0
1	MLY	A	288	1	-	0/5/7/11	0/0/0/0
1	MLY	A	3	1	-	0/5/7/11	0/0/0/0
1	MLY	A	324	1	-	0/7/9/11	0/0/0/0
1	MLY	A	47	1	-	0/0/2/11	0/0/0/0
1	MLY	A	5	1	-	0/7/9/11	0/0/0/0
1	MLY	A	70	1	-	0/2/4/11	0/0/0/0
1	MLY	A	74	1	-	0/0/2/11	0/0/0/0
1	MLY	B	116	1	-	0/5/7/11	0/0/0/0
1	MLY	B	123	1	-	0/7/9/11	0/0/0/0
1	MLY	B	20	1	-	0/5/7/11	0/0/0/0
1	MLY	B	205	1	-	0/3/5/11	0/0/0/0
1	MLY	B	215	1	-	0/2/4/11	0/0/0/0
1	MLY	B	25	1	-	0/7/9/11	0/0/0/0
1	MLY	B	261	1	-	0/7/9/11	0/0/0/0
1	MLY	B	288	1	-	0/2/4/11	0/0/0/0
1	MLY	B	3	1	-	0/5/7/11	0/0/0/0
1	MLY	B	5	1	-	0/5/7/11	0/0/0/0
1	MLY	B	70	1	-	0/7/9/11	0/0/0/0
1	MLY	B	74	1	-	0/5/7/11	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	MLY	O-C	20.23	1.25	1.11
1	B	288	MLY	O-C	19.10	1.24	1.11
1	A	5	MLY	O-C	19.04	1.24	1.11
1	A	20	MLY	O-C	18.76	1.24	1.11
1	A	70	MLY	O-C	18.65	1.24	1.11
1	A	324	MLY	O-C	18.46	1.24	1.11
1	A	47	MLY	O-C	18.46	1.24	1.11
1	A	3	MLY	O-C	18.38	1.24	1.11
1	A	25	MLY	O-C	18.24	1.24	1.11
1	B	74	MLY	O-C	18.06	1.23	1.11
1	A	74	MLY	O-C	18.06	1.23	1.11
1	B	116	MLY	O-C	17.90	1.23	1.11
1	A	215	MLY	O-C	17.50	1.23	1.11

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	123	MLY	O-C	17.43	1.23	1.11
1	A	205	MLY	O-C	17.39	1.23	1.11
1	B	20	MLY	O-C	17.36	1.23	1.11
1	A	116	MLY	O-C	17.07	1.23	1.11
1	B	25	MLY	O-C	17.03	1.23	1.11
1	B	3	MLY	O-C	16.73	1.22	1.11
1	B	215	MLY	O-C	16.58	1.22	1.11
1	B	261	MLY	O-C	15.88	1.22	1.11
1	B	70	MLY	O-C	15.61	1.22	1.11
1	A	123	MLY	O-C	15.25	1.21	1.11
1	A	261	MLY	O-C	15.10	1.21	1.11
1	B	205	MLY	O-C	14.78	1.21	1.11
1	A	288	MLY	O-C	13.38	1.20	1.11
1	A	20	MLY	CG-CB	4.48	1.56	1.55
1	A	70	MLY	CG-CB	-3.86	1.53	1.55
1	B	205	MLY	CD-CG	-3.18	1.53	1.55
1	A	324	MLY	CB-CA	2.86	1.55	1.53
1	B	288	MLY	CG-CB	-2.57	1.54	1.55
1	B	288	MLY	CA-C	2.39	1.52	1.48
1	B	215	MLY	CG-CB	-2.36	1.54	1.55
1	A	116	MLY	CA-C	2.34	1.52	1.48
1	A	288	MLY	CA-C	2.23	1.52	1.48
1	A	47	MLY	CA-C	2.16	1.52	1.48
1	B	215	MLY	CA-C	2.12	1.52	1.48
1	B	70	MLY	CA-C	2.08	1.52	1.48
1	A	3	MLY	CA-C	2.07	1.52	1.48
1	A	5	MLY	CA-C	2.07	1.52	1.48
1	B	205	MLY	CB-CA	2.02	1.55	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	MLY	C-CA-N	-7.23	106.61	113.83
1	B	5	MLY	C-CA-N	-5.97	107.86	113.83
1	A	74	MLY	C-CA-N	-5.25	108.59	113.83
1	A	25	MLY	C-CA-N	-4.66	109.17	113.83
1	B	3	MLY	C-CA-N	-4.63	109.21	113.83
1	A	25	MLY	CH2-NZ-CH1	4.36	121.62	109.75
1	A	288	MLY	C-CA-N	-4.14	109.69	113.83
1	A	324	MLY	CH2-NZ-CH1	4.07	120.82	109.75
1	B	116	MLY	C-CA-N	-3.98	109.85	113.83
1	B	261	MLY	C-CA-N	-3.98	109.86	113.83

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	MLY	CH2-NZ-CH1	3.92	120.43	109.75
1	A	5	MLY	CH2-NZ-CH1	3.77	120.00	109.75
1	A	3	MLY	C-CA-N	-3.63	110.20	113.83
1	A	123	MLY	C-CA-N	-3.54	110.30	113.83
1	B	123	MLY	CH2-NZ-CH1	3.52	119.31	109.75
1	B	261	MLY	CH2-NZ-CH1	3.49	119.25	109.75
1	A	205	MLY	CH2-NZ-CH1	3.37	118.92	109.75
1	A	261	MLY	CH2-NZ-CH1	3.35	118.86	109.75
1	B	70	MLY	CH2-NZ-CH1	3.30	118.72	109.75
1	B	25	MLY	C-CA-N	-3.09	110.74	113.83
1	A	205	MLY	CH2-NZ-CE	2.76	122.13	110.76
1	B	261	MLY	CH2-NZ-CE	2.76	122.11	110.76
1	B	70	MLY	C-CA-N	-2.72	111.11	113.83
1	A	25	MLY	CH2-NZ-CE	2.69	121.83	110.76
1	A	324	MLY	CH1-NZ-CE	2.64	121.63	110.76
1	B	123	MLY	C-CA-N	-2.64	111.19	113.83
1	B	70	MLY	CH2-NZ-CE	2.54	121.22	110.76
1	B	25	MLY	CH1-NZ-CE	2.53	121.20	110.76
1	A	261	MLY	CH1-NZ-CE	2.49	121.02	110.76
1	A	5	MLY	CH1-NZ-CE	2.44	120.81	110.76
1	B	3	MLY	CB-CA-N	2.41	117.73	110.67
1	B	123	MLY	CH2-NZ-CE	2.41	120.70	110.76
1	A	261	MLY	CH2-NZ-CE	2.27	120.10	110.76
1	B	70	MLY	CH1-NZ-CE	2.26	120.06	110.76
1	B	123	MLY	CH1-NZ-CE	2.23	119.97	110.76
1	B	205	MLY	CD-CG-CB	-2.23	109.44	114.46
1	A	261	MLY	C-CA-N	-2.17	111.66	113.83
1	B	205	MLY	CG-CB-CA	-2.11	110.49	114.43
1	A	5	MLY	CD-CE-NZ	-2.07	108.17	113.59
1	A	5	MLY	CH2-NZ-CE	2.04	119.18	110.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	PEG	A	327	-	6,6,6	0.83	0	5,5,5	0.65	0
3	PEG	A	328	-	6,6,6	0.69	0	5,5,5	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	A	327	-	-	0/4/4/4	0/0/0/0
3	PEG	A	328	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	316/326 (96%)	0.40	26 (8%) 12 11	24, 37, 64, 92	0
1	B	305/326 (93%)	0.44	30 (9%) 8 7	26, 43, 69, 88	0
All	All	621/652 (95%)	0.42	56 (9%) 10 9	24, 40, 69, 92	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	323	VAL	6.3
1	A	41	SER	6.1
1	A	48	ASN	5.8
1	B	10[A]	GLY	5.5
1	B	304	GLY	5.5
1	B	1	MSE	5.4
1	A	1	MSE	4.9
1	A	55	PRO	4.8
1	B	37	ASP	4.5
1	B	188	VAL	4.3
1	B	275	TYR	4.2
1	A	42	SER	4.2
1	A	92	LEU	4.2
1	A	87	PHE	4.0
1	A	88	ALA	4.0
1	B	9	ILE	3.9
1	B	189	LEU	3.9
1	B	87	PHE	3.6
1	A	40	GLY	3.5
1	A	9	ILE	3.5
1	A	81	SER	3.4
1	B	8	VAL	3.4
1	B	303	ASN	3.3
1	B	301	LEU	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	270	ASN	3.2
1	A	202	ILE	3.2
1	A	270	ASN	3.1
1	A	303	ASN	3.1
1	B	266	TYR	3.0
1	B	302	GLU	2.9
1	B	221	VAL	2.9
1	B	272	PHE	2.9
1	B	187	ILE	2.9
1	A	43	GLY	2.9
1	B	220	TYR	2.8
1	B	12	GLY	2.7
1	A	79	ARG	2.7
1	B	219	ALA	2.6
1	B	11[A]	GLY	2.6
1	A	198	ILE	2.5
1	B	76	PHE	2.5
1	B	191	PRO	2.5
1	B	190	GLY	2.5
1	B	198	ILE	2.4
1	A	90	HIS	2.4
1	A	80	PHE	2.4
1	A	302	GLU	2.4
1	A	304	GLY	2.4
1	A	166	LEU	2.3
1	A	189	LEU	2.2
1	B	15[A]	SER	2.2
1	B	271	ARG	2.1
1	A	305	GLY	2.1
1	A	199	LEU	2.0
1	A	121	THR	2.0
1	B	305	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	288	9/12	0.17	5.50	29,31,49,60	0
1	MLY	A	261	11/12	0.16	2.98	28,35,58,64	0
1	MLY	B	288	6/12	0.20	1.95	41,43,43,43	0
1	MLY	B	70	11/12	0.24	1.85	32,38,75,77	0
1	MLY	A	74	5/12	0.16	1.70	44,46,50,53	0
1	MLY	A	3	9/12	0.27	1.62	41,51,65,68	0
1	MLY	B	116	9/12	0.13	1.16	35,42,51,57	0
1	MLY	B	123	11/12	0.16	0.96	38,46,76,81	0
1	MLY	A	324	11/12	0.17	0.71	34,40,48,51	0
1	MLY	B	25	11/12	0.15	0.62	39,43,64,69	0
1	MLY	A	205	11/12	0.15	0.29	27,32,72,73	0
1	MLY	B	20	9/12	0.18	0.28	38,41,59,62	0
1	MLY	B	261	11/12	0.18	0.01	41,43,58,61	0
1	MLY	B	215	6/12	0.10	-0.20	35,35,36,39	0
1	MLY	A	116	9/12	0.11	-0.43	33,34,42,43	0
1	MLY	A	47	5/12	0.16	-0.62	66,69,73,74	0
1	MLY	B	3	9/12	0.12	-0.67	45,54,65,68	0
1	MLY	A	20	6/12	0.10	-0.69	37,39,41,43	0
1	MLY	A	5	11/12	0.09	-0.74	29,38,66,69	0
1	MLY	A	25	11/12	0.10	-0.76	39,41,67,68	0
1	MLY	B	74	9/12	0.10	-0.78	44,46,50,53	0
1	MLY	B	5	9/12	0.12	-0.79	37,39,47,53	0
1	MLY	A	215	9/12	0.10	-0.80	25,27,40,51	0
1	MLY	A	123	6/12	0.07	-1.31	36,39,44,46	0
1	MLY	B	205	7/12	0.09	-1.81	32,34,42,54	0
1	MLY	A	70	6/12	0.08	-1.85	40,40,42,49	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	A	328	7/7	0.21	4.48	52,60,69,73	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	A	327	7/7	0.15	1.45	29,57,63,66	0
2	CL	A	326	1/1	0.05	-4.08	38,38,38,38	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.